

Wildfire Impacts on Ozone on June 21, 2015 at the El Paso UTEP Monitoring Site

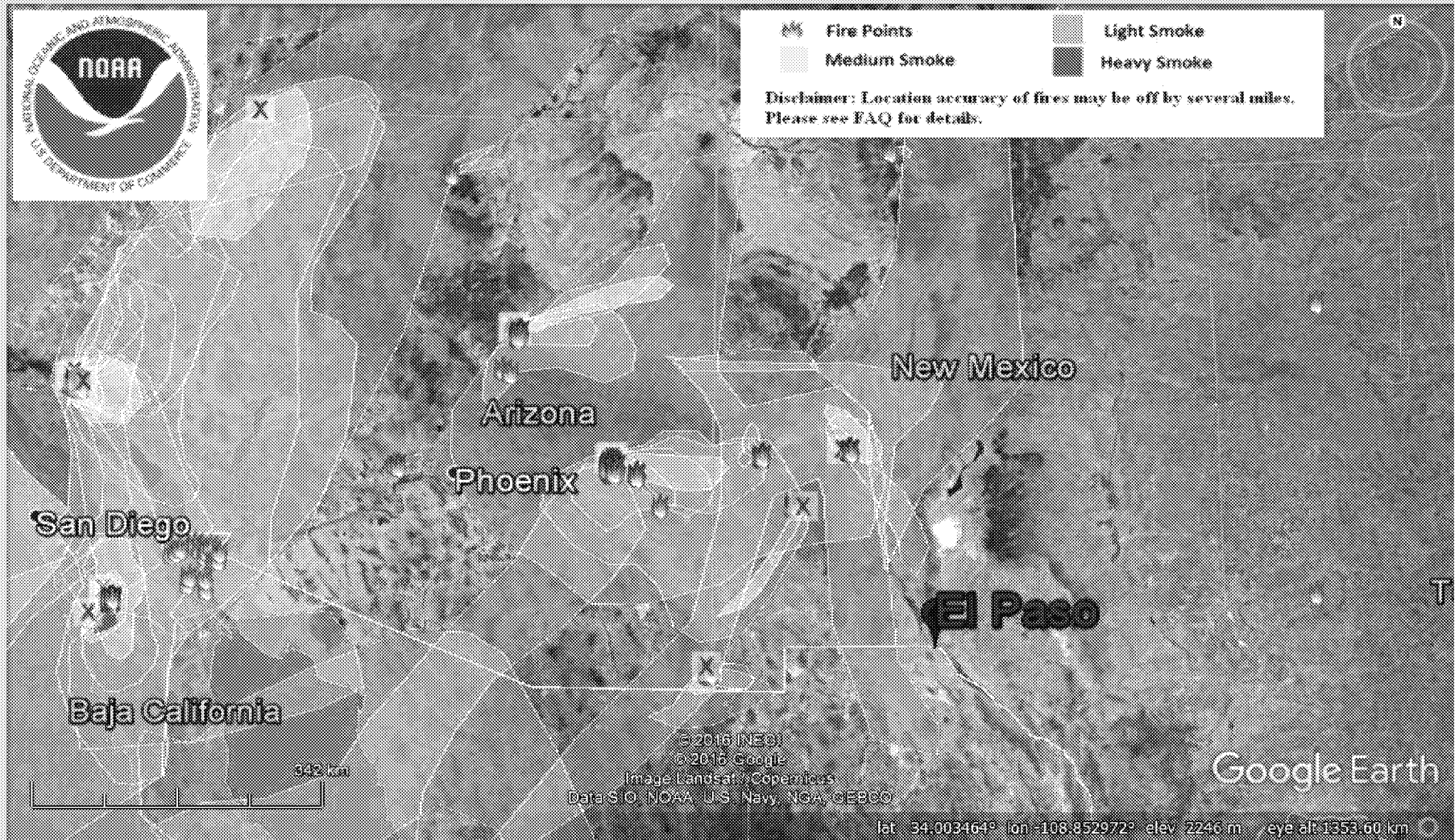
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Presented at U.S. EPA Region 6
May 22, 2017

Key points

- Fires and smoke were present in the area. Prior TCEQ documentation and CAMx modeling demonstrates transport to El Paso UTEP site on June 21.
- Diurnal pattern of $PM_{2.5}$ on June 21 in El Paso was unusual and consistent with fire plumes and the CAMx modeling.
- Ratio of O_3 to $PM_{2.5}$ was consistent with published studies on O_3 production.
- I used a Generalized Additive Model to predict hourly O_3 with an R^2 of 0.645. Model residuals are unbiased with respect to model prediction levels and time of day. Model was further evaluated by excluding individual years of data and recalculated to examine fit for years that were excluded.
- Our best estimate of the contribution to the MDA8 from the fires is 23 ppb. Following the EPA guidance we calculate a minimum contribution of 7 ppb.

NOAA HMS Fire and Smoke Product show extensive smoke in the area on June 20-21, 2015



KMZ files are here:

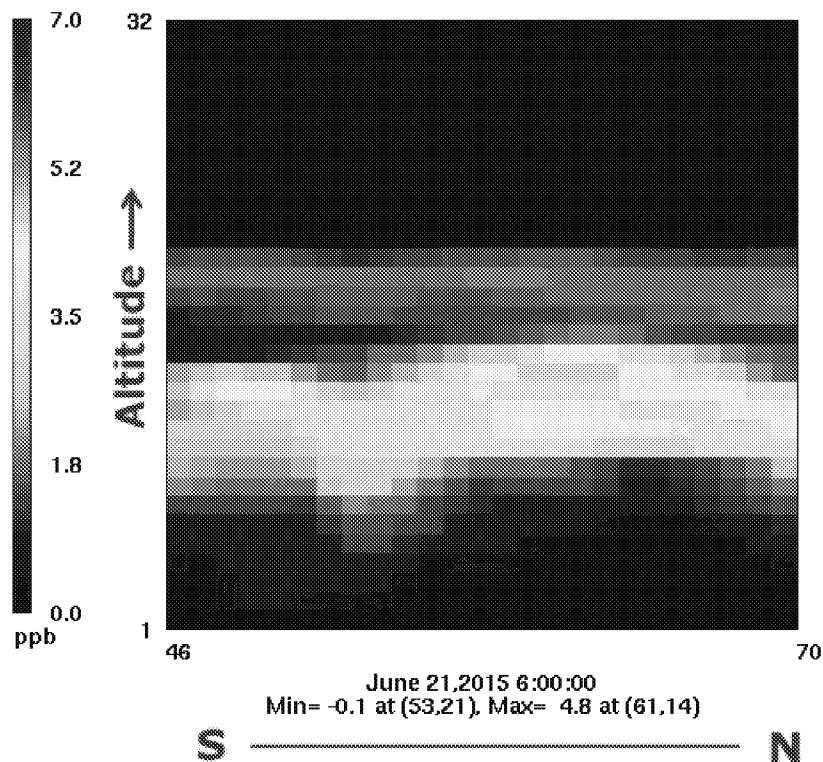
<ftp://satepsanone.nesdis.noaa.gov/FIRE/HMS/KML/ARCHIVE/>

CAMX modeling demonstrates transport and mixing down to surface

Ozone Cross Section

1-Hour Average Ozone from Fires

North-South Vertical Cross Section Above UTEP CAMS 12
June 17-22, 2015

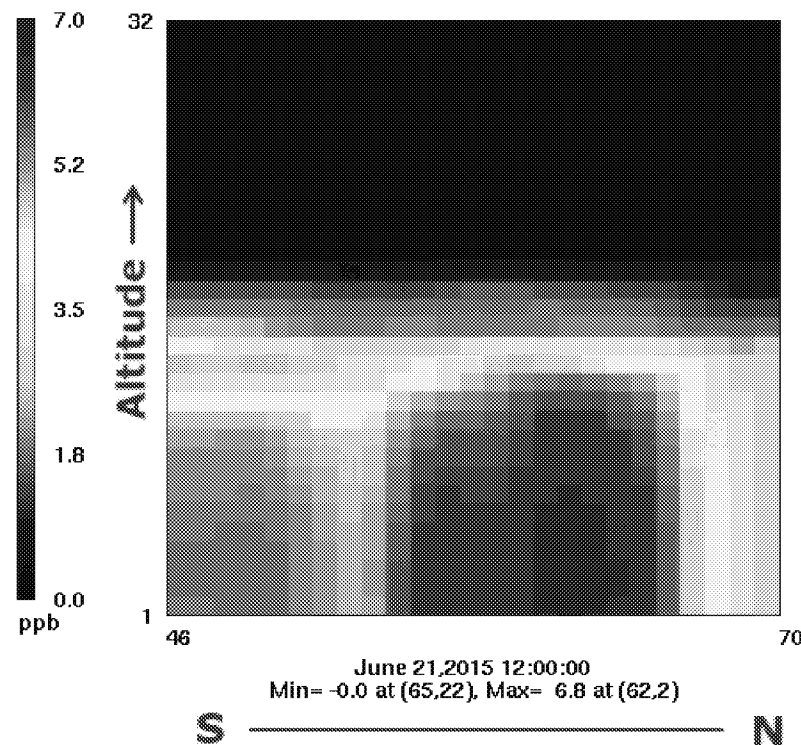


June 21, 2015, 600 am

Ozone Cross Section

1-Hour Average Ozone from Fires

North-South Vertical Cross Section Above UTEP CAMS 12
June 17-22, 2015



June 21, 2015, 12 noon

Kemball-Cook and Johnson, Ramboll-Environ 2017

Summary of $\Delta\text{O}_3/\Delta\text{CO}$ from >100 published studies

Boreal/ Temperate:

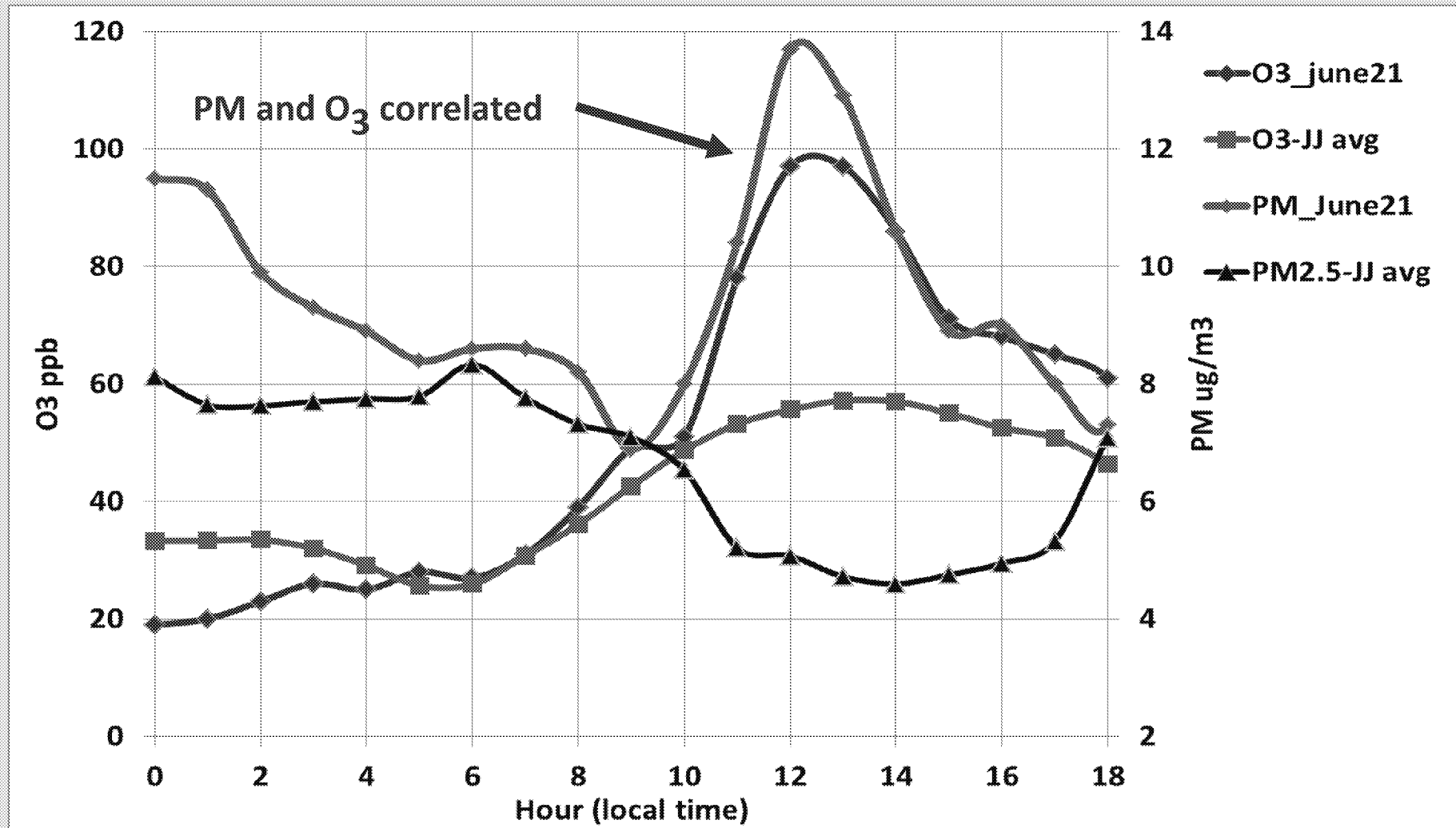
Plume Age	Mean $\Delta\text{O}_3/\Delta\text{CO}$ (ppbv/ppbv) (# plumes)	Range of $\Delta\text{O}_3/\Delta\text{CO}$
$\leq 1\text{-}2$ days	0.018 (n=55)	-0.032-0.34
2-5 days	0.15 (n=39)	-0.07-0.66
≥ 5 days	0.22 (n=29)	-0.42-0.93

Tropics/ Subtropics:

Plume Age	Mean $\Delta\text{O}_3/\Delta\text{CO}$ (ppbv/ppbv) (# plumes)	Range of $\Delta\text{O}_3/\Delta\text{CO}$
$\leq 1\text{-}2$ days	0.14 (n=59)	-0.06-0.37
2-5 days	0.35 (n=13)	0.26-0.42
≥ 5 days	0.63 (n=18)	0.19-0.87

Jaffe, D.A. and Wigder, N.L., Ozone production from wildfires: A critical review. Atmos. Envir., doi:10.1016/j.atmosenv.2011.11.063, 2012.

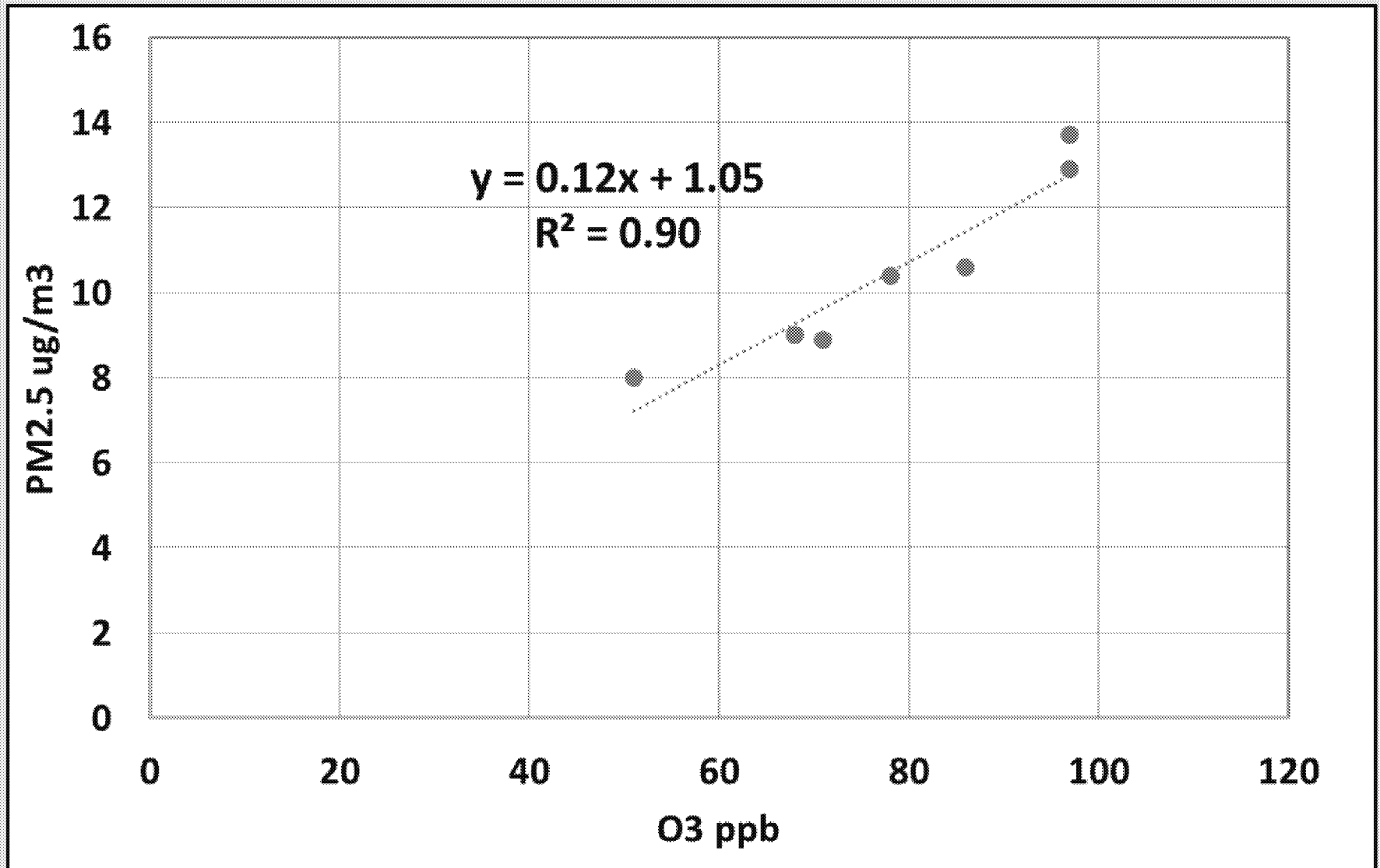
PM and O₃ data for June 21, 2015; MDA8 = 77 ppb



Hourly PM and O₃ data for June 21 are shown along with all hourly data from June-July 2015. Normal pattern is for PM to be high at night and O₃ during day with no correlation between the two. On June 21, PM and O₃ are in sync between hours 10-14. This is different from usual pattern and suggests a smoke plume passed over El Paso and mixed to ground level.

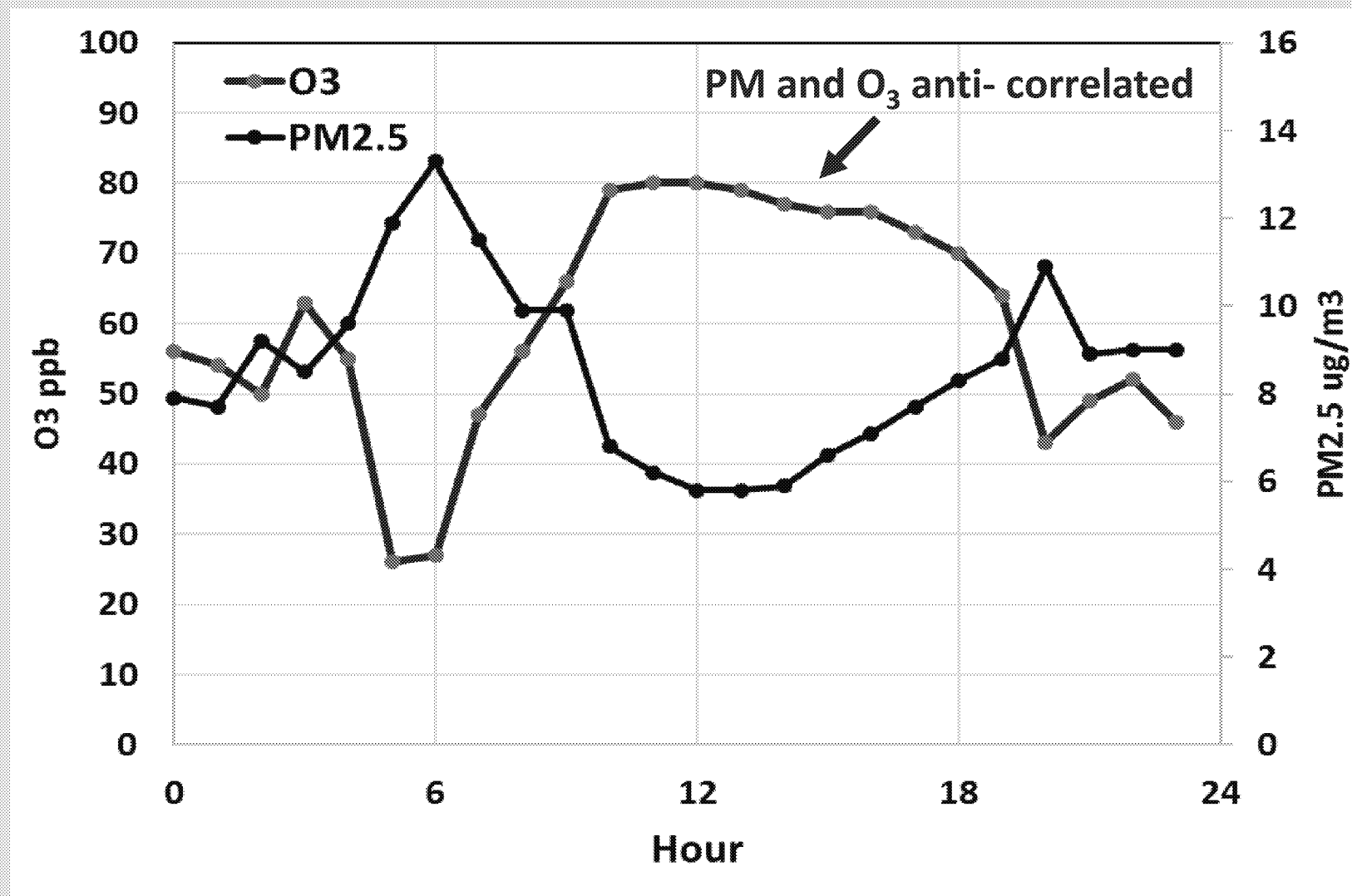
PM and O₃ well correlated on June 21, 2015

Using hourly data 10am-5 pm



**Are PM and O₃ correlated on other
high O₃ days?**

PM and O₃ data for July 13, 2012; MDA8 = 77 ppb



This is the more typical pattern; higher PM at night and high O₃ in day.

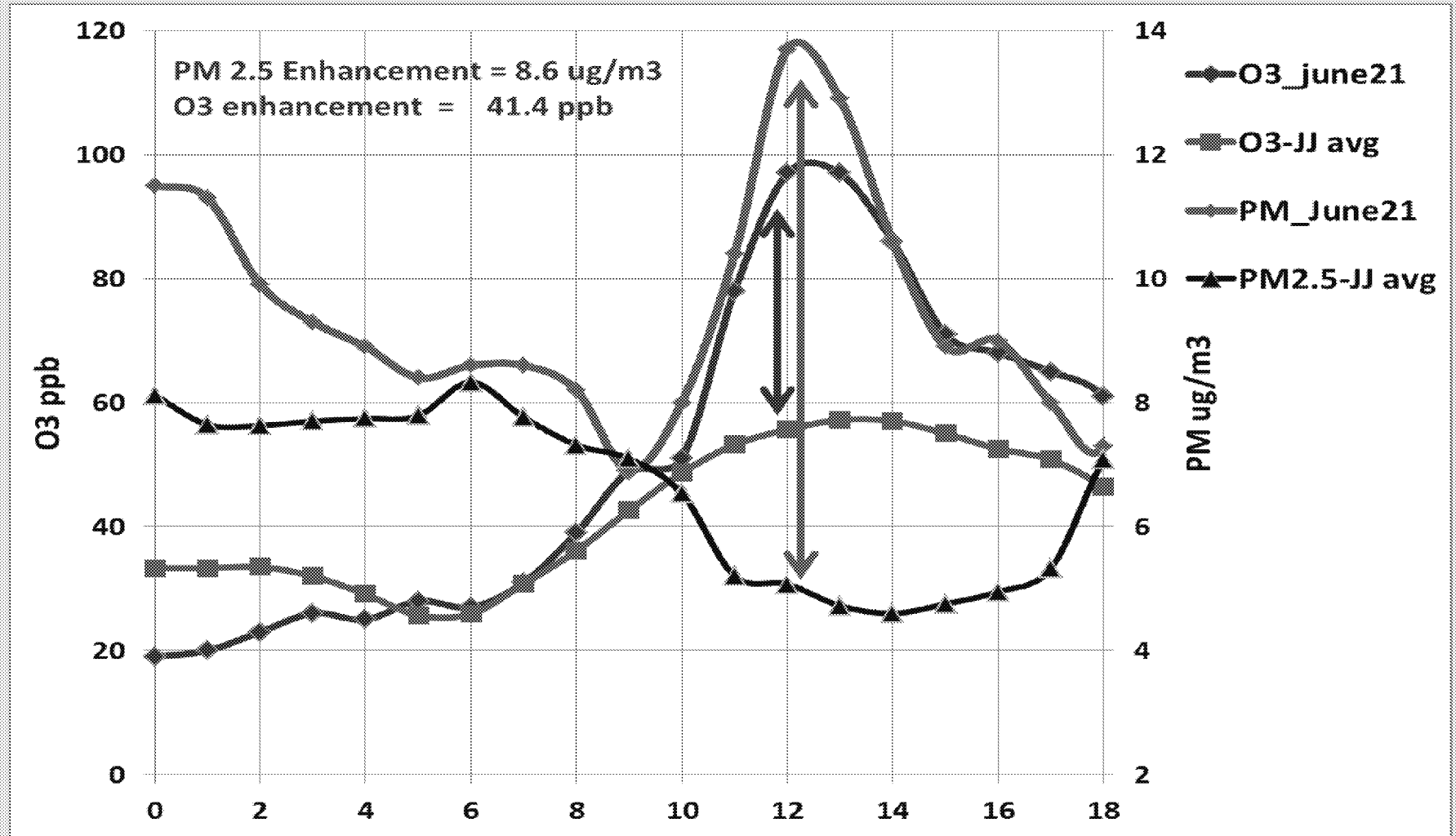
**PM_{2.5}-O₃ relationship for all days with MDA8>70 for 2010-2015
(daily 10 am – 5 pm data, N=31)
Need R² > 0.66 for statistical significance (P<.05)**

Date	MDA8 (ppb)	O ₃ /PM _{2.5} SLOPE (ppb per ug/m ³)	R ²	Date	MDA8 (ppb)	O ₃ /PM _{2.5} SLOPE (ppb per ug/m ³)	R ²
7/13/2010	87	-3.8	0.26	8/10/2015	74	2.3	0.11
7/3/2013	82	-4.2	0.12	8/10/2010	73	-3.2	0.25
7/19/2010	81	2.7	0.17	4/28/2013	73	-0.7	0.06
6/17/2015	81	3.4	0.2	8/17/2013	73	-2	0.29
6/4/2011	78	3.4	0.49	8/19/2013	73	1.5	0.02
6/22/2011	78	-1.7	0.7	6/10/2014	73	6.5	0.4
7/13/2012	77	-2.8	0.61	7/15/2010	72	-2	0.06
6/21/2015	77	7.1	0.9	6/28/2012	72	-1.8	0.6
7/12/2012	75	2.1	0.57	7/14/2012	72	4.7	0.52
5/24/2013	75	2.8	0.47	6/21/2014	72	6	0.6
6/11/2013	75	0	0	6/29/2015	72	-1.6	0.01
7/15/2014	75	-0.1	0	7/20/2011	71	0.7	0
8/20/2010	74	-8	0.26	6/29/2012	71	-1.3	0.13
8/4/2012	74	5.3	0.3	8/12/2012	71	0.6	0.05
8/31/2012	74	1.1	0	8/21/2012	71	4.7	0.44
9/2/2012	74	0.8	0.06				

6/21/2015 is the only day with a statistically significant positive PM-O₃ correlation.

**Is the PM- O₃ enhancement ratio
consistent with a wildfire source?**

Analysis of June 21, 2015 event



Arrows show method to calculate enhancement ratio of $\text{PM}_{2.5}$ and O_3 on June 21.
The $\Delta\text{O}_3/\Delta\text{PM}_{2.5}$ enhancement ratio is 4.8 ppb of O_3 per $\mu\text{g}/\text{m}^3$ of $\text{PM}_{2.5}$.

Is the enhancement ratio of 4.8 ppb of O₃ per µg/m³ of PM_{2.5} consistent with a wildfire source?

- Limited information in literature directly comparing PM to O₃. This is because PM and O₃ are often uncorrelated in fresh plumes.
- Instead use data for aged plumes (2 or more days since emissions):

$$\frac{\Delta O_3}{\Delta PM_{2.5}} = \frac{\Delta O_3}{\Delta CO} * \frac{\Delta CO}{\Delta PM_{2.5}}$$

- Laing et al (2017) reports $\Delta PM_{2.5}/\Delta CO$ in 25 different wildfire events as seen at 8 urban locations in the Western U.S. Average $\Delta PM_{2.5}/\Delta CO = 0.13 \mu\text{g}/\text{m}^3$ per ppb, with a range of CO range of 0.06-0.23. These values are consistent with known emission ratios (Akagi et al 2011).
- Invert to get $\Delta CO/\Delta PM_{2.5}$ ratios of 7.7, 16.7 and 4.3 respectively.
- Jaffe and Wigder review >100 published studies on aged fire plumes and report mean, min and max values for $\Delta O_3/\Delta CO$ of 0.35, 0.26 and 0.42, respectively for sub-tropical wildfire plumes aged 2-5 days.
- Combine these to estimate a range for $\Delta O_3/\Delta PM_{2.5}$.

$$\frac{\Delta O_3}{\Delta PM_{2.5}} = \frac{\Delta O_3}{\Delta CO} * \frac{\Delta CO}{\Delta PM_{2.5}}$$

Mean value:

$$\frac{\Delta O_3}{\Delta PM_{2.5}} = 0.35 * 7.7 = 2.7 \frac{ppb}{ug \text{ per } m^3}$$

Maximum value:

$$\frac{\Delta O_3}{\Delta PM_{2.5}} = 0.42 * 16.7 = 7.0 \frac{ppb}{ug \text{ per } m^3}$$

Minimum value:

$$\frac{\Delta O_3}{\Delta PM_{2.5}} = 0.26 * 4.3 = 1.1 \frac{ppb}{ug \text{ per } m^3}$$

The June 21, 2015 enhancement ratio ($\Delta O_3/\Delta PM_{2.5}$) of 4.8 ppb per $\mu g/m^3$ falls within this range.

Summary of PM_{2.5}-O₃ relationship

- CAMx modeling indicates transport of smoke to El Paso on June 21.
- The pattern of PM_{2.5} on this day is consistent with transport of smoke over El Paso, followed by mixing into the boundary layer in the mid-day.
- Enhanced PM_{2.5} and O₃ occurred simultaneously and were significantly correlated ($R^2=0.9$) between 10 am -5 pm. This was the only high O₃ day in the 2010-2015 time period with a statistically significant and positive correlation between PM_{2.5} and O₃.
- By comparing the hourly data for June 21, with the usual pattern we can calculate the enhancement in PM_{2.5} and O₃ for this day. O₃ was enhanced by 41.4 ppb, PM_{2.5} by 8.6 ug/m³ or 4.8 ppb of O₃ per ug/m³ of PM_{2.5}.
- Published data for this enhancement ratio indicates a range of between 1 and 7 ppb of O₃ per ug/m³ of PM_{2.5} for wildfire plumes aged more than 1 day. The June 21st value is within this range.
- Therefore I conclude the transport modeling, pattern of PM_{2.5}, the PM_{2.5}-O₃ correlation and the $\Delta O_3/\Delta PM_{2.5}$ enhancement ratio are all consistent with smoke from wildfires as a significant contributor to the mid-day peak in O₃ on June 21, 2015.
- Next I estimate the amount of O₃ contributed by the wildfires.

Eulerian modeling vs Statistical modeling

Eulerian modeling (e.g. CAMx):

- Gridded emissions, meteorology, solar fluxes (J values).
- Use known photochemistry and transport to model mixing ratios.
- For wildfires significant challenges with emissions, plume rise, aerosols and the chemistry, which can be very different from typical urban photochemistry.
- Modeled concentrations may differ significantly from observations making quantitative attribution difficult (e.g. see Baker et al 2016).

Statistical modeling (e.g. GAM used in this work):

- Examines the relationship between observed mixing ratios and other factors.
- Possible factors to include are temp, wind speed, RH, solar flux, etc.
- Outliers (high residuals) represent an additional O₃ source and are candidates for further investigation.

$$O_3 = A * \text{temp} + B * \text{winds} + C * \text{DOY} \dots + \text{residual}$$

(A,B,C are “link” functions)

Jaffe et al 2004; 2013; Camalier et al 2007; CARB 2011; EPA 2015; Sun et al 2015

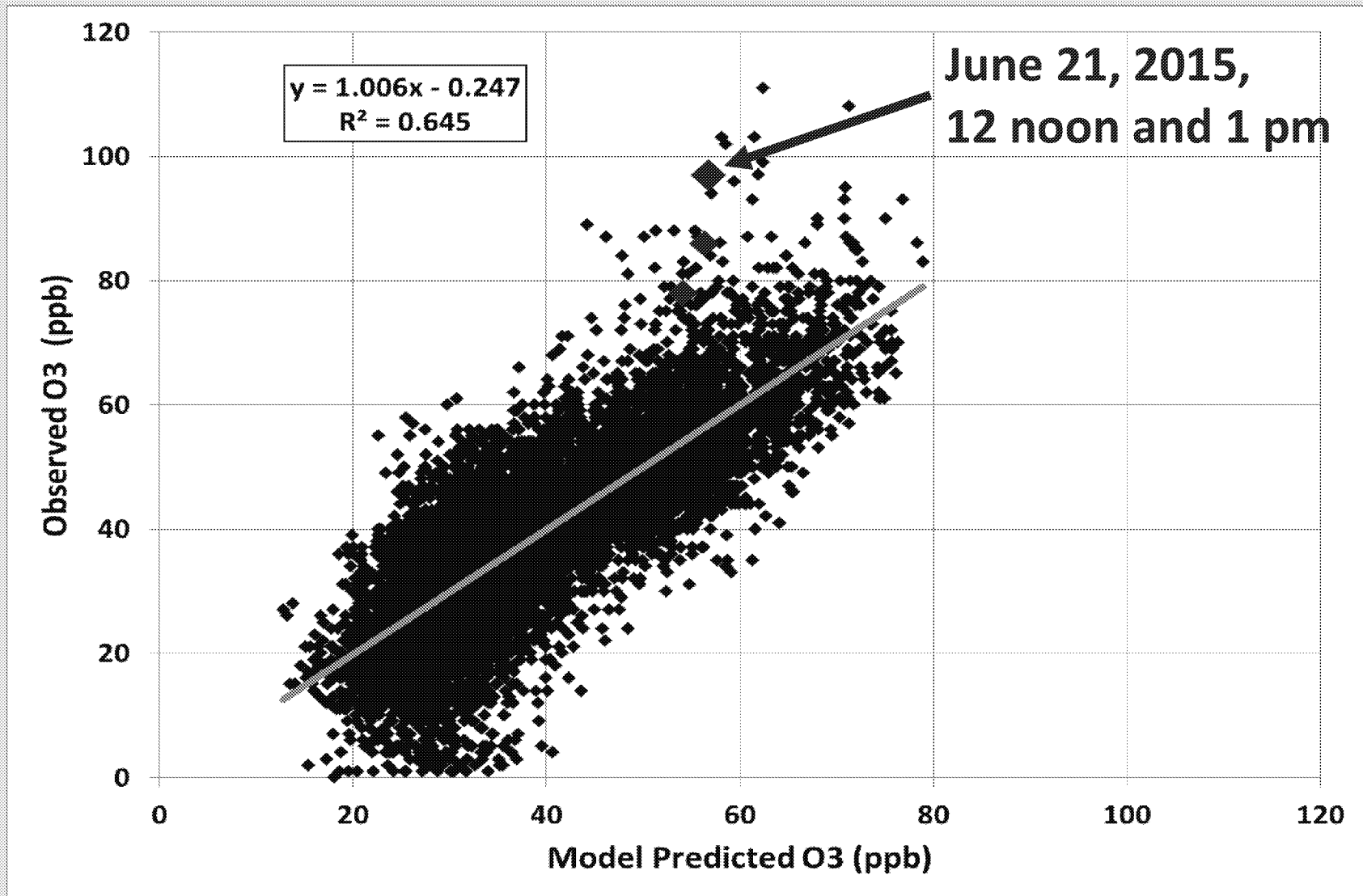
Strategy for Statistical Modeling

- Use data from May-Sept 2011-2015.
- Use Generalized Additive Model on hourly UTEP O_3 data.
- GAM allows for non-linear relationships and categorical (non-numerical) variables.
- Use “gam” function in R software with mgcv package with Log-link function and Gaussian error distribution.

Predictors for El Paso Generalized Additive Model (GAM)

Description	Source	Variable Type Categorical or Numeric
Back-trajectory quadrant after 24 hours	NOAA Hysplit	C
Month	Month	C
Vector averaged wind direction for hours 0-17	NCDC	C
Year	Year	N
Day of Year	Day of Year	N
Back-trajectory distance after 24 hours	NOAA Hysplit	N
Hour of day	Hour of day	N
Daily max temperature	NCDC	N
Daily average temperature	NCDC	N
Min temperature previous night	NCDC	N
Daily average dew point	NCDC	N
Daily maximum dew point for hours 0-17	NCDC	N
Daily minimum dew point for hours 0-17	NCDC	N
Daily average sea level pressure	NCDC	N
Daily average sea level pressure for hours 0-17	NCDC	N
Vector averaged wind speed for hours 0-17	NCDC	N
Vector averaged wind speed for hours 6-17	NCDC	N
Vector averaged wind speed for hours 10-17	NCDC	N

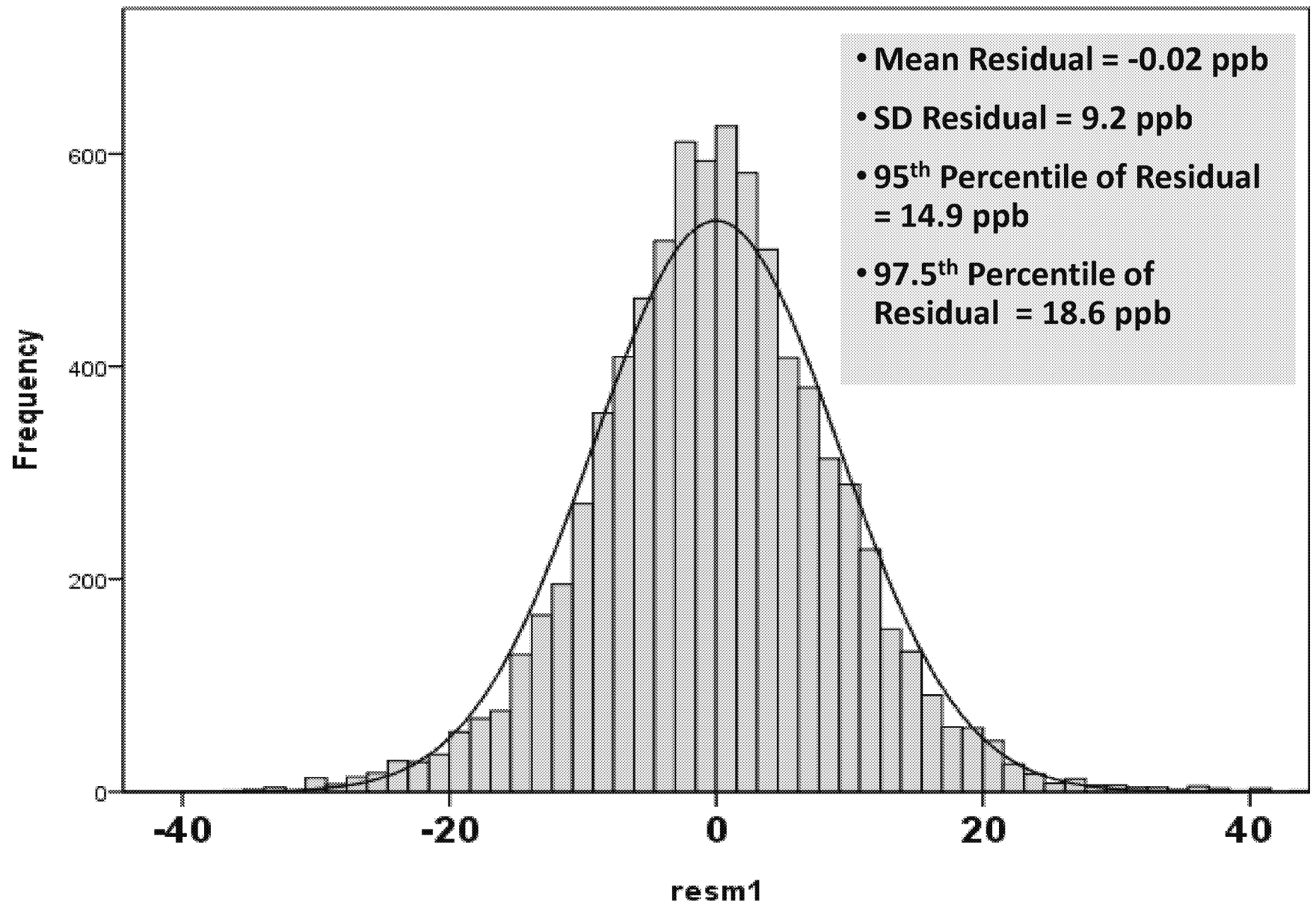
Model performance



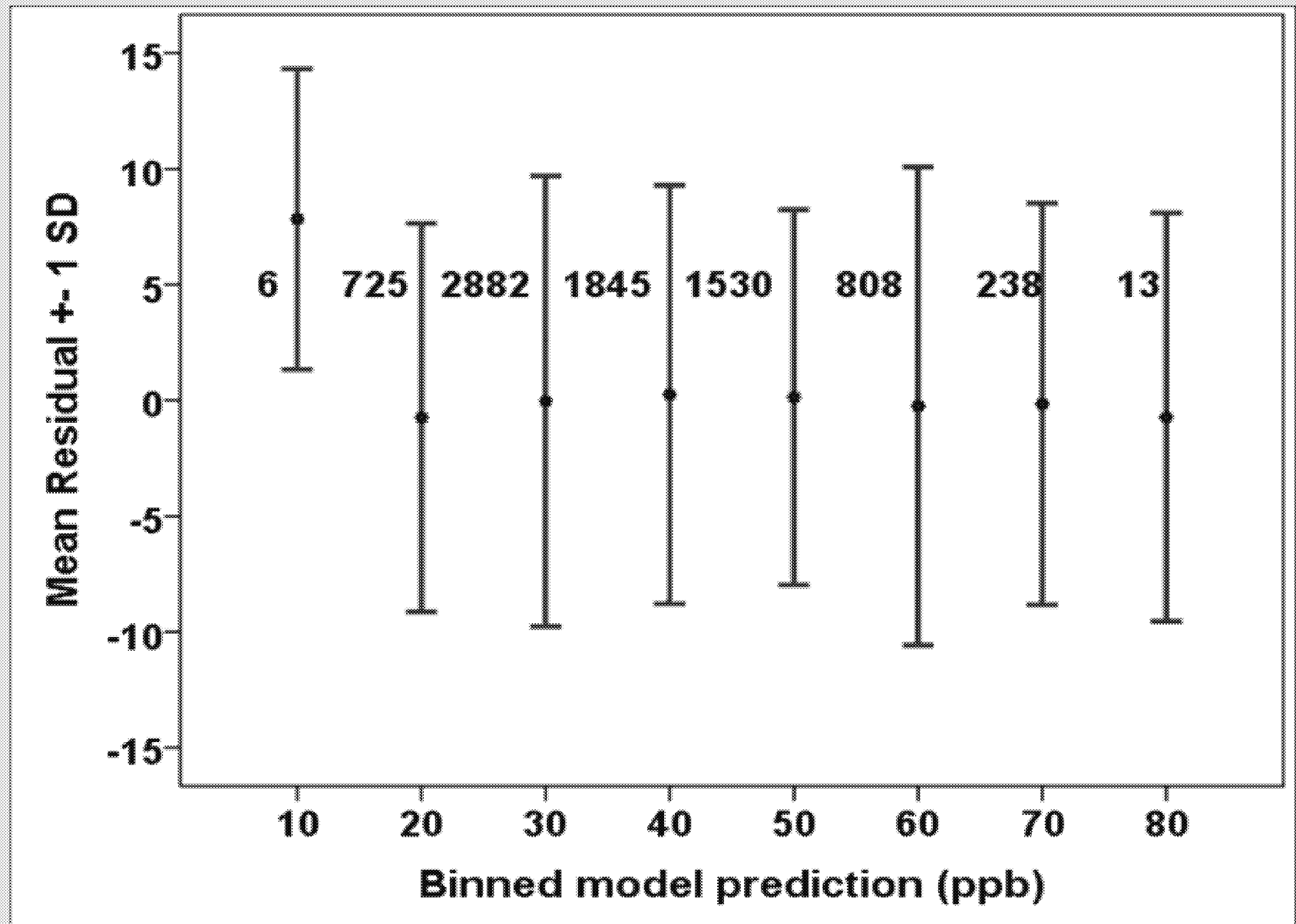
Points for June 21, 2015 hours 11 am-2pm are shown in red.
Larger symbols indicates two points (12 noon and 1 pm)

Model Evaluation

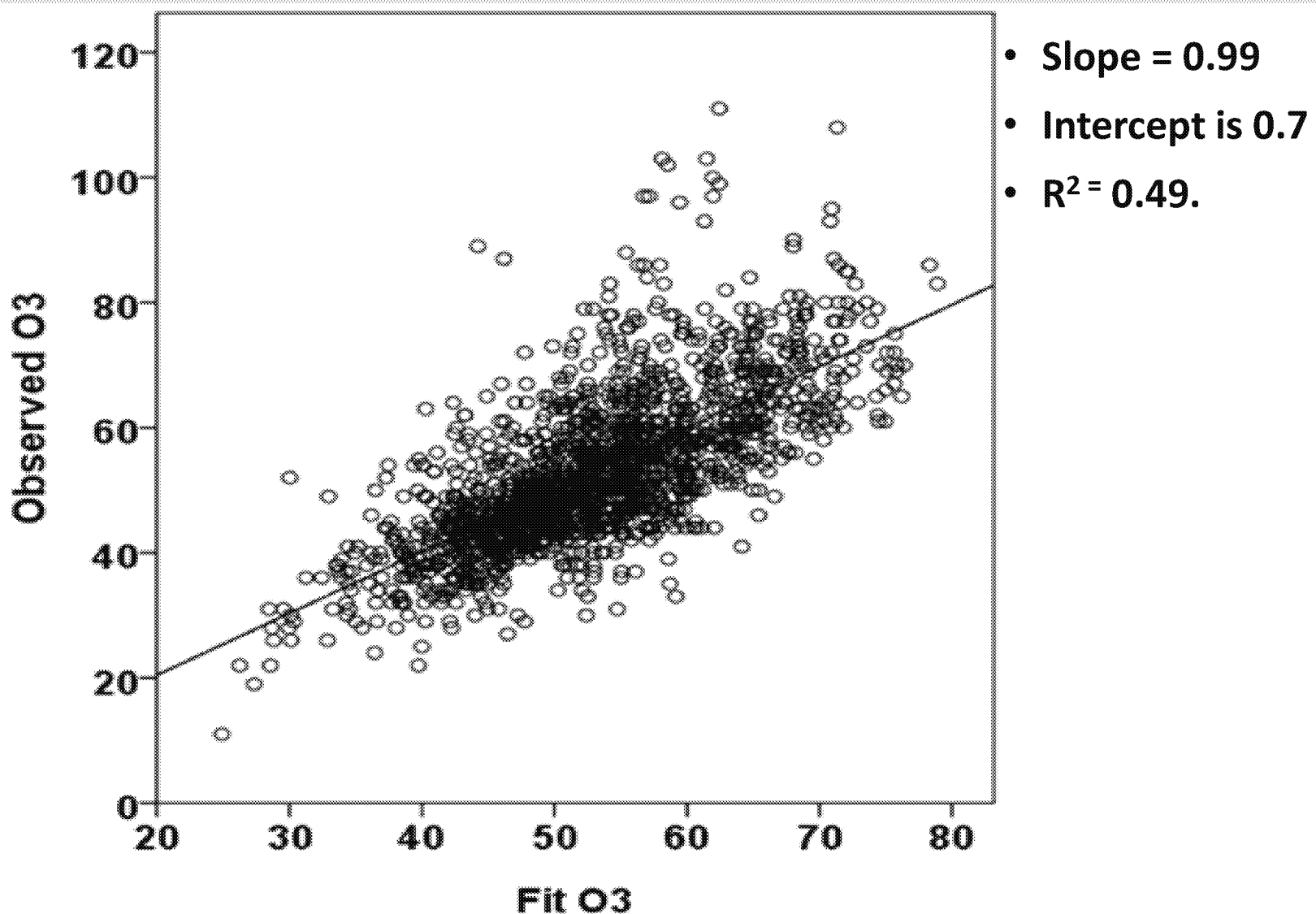
Model residuals (observed-fit, ppb)



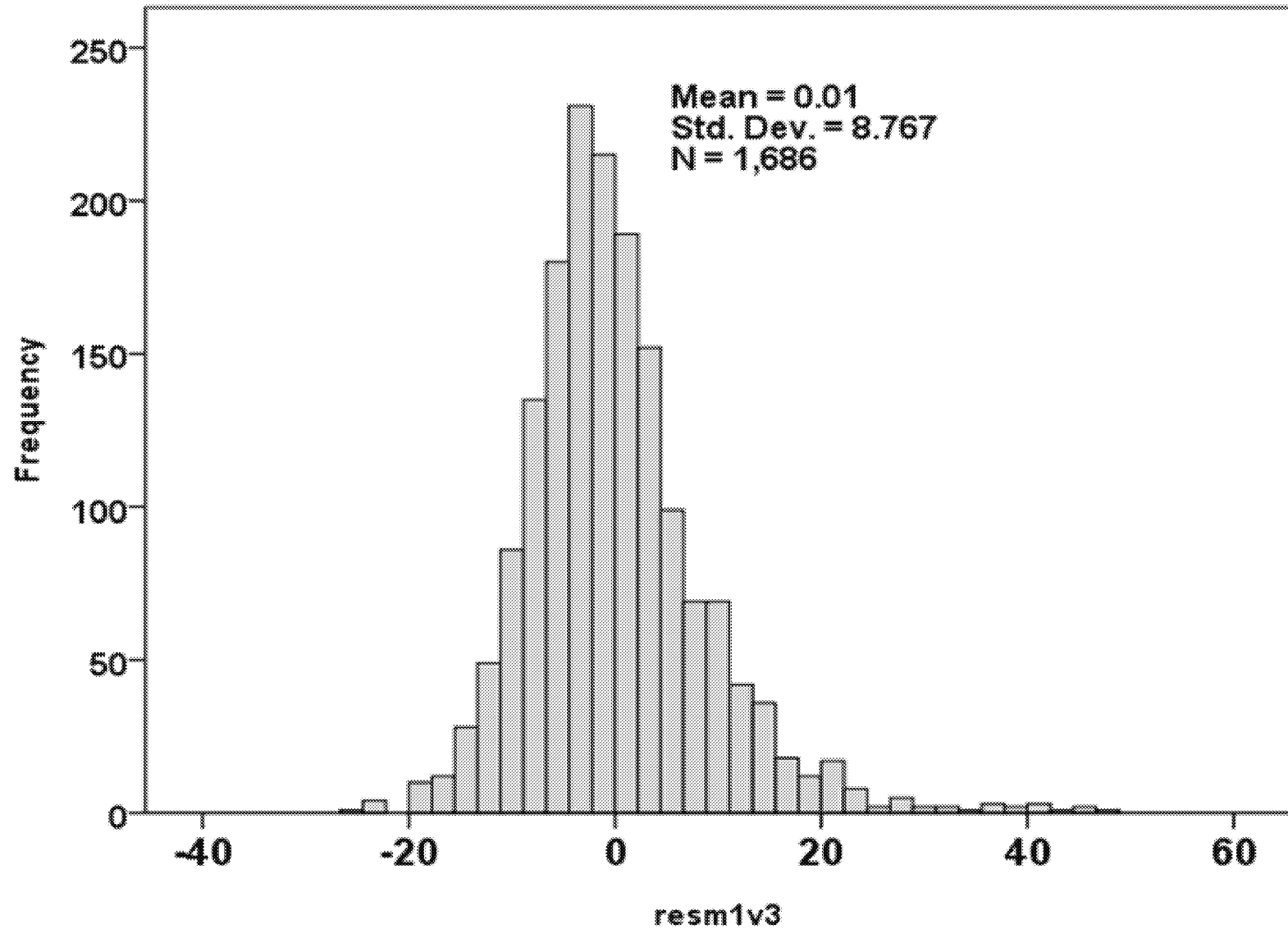
Model residuals vs Model prediction (Bars show SD, values give N)



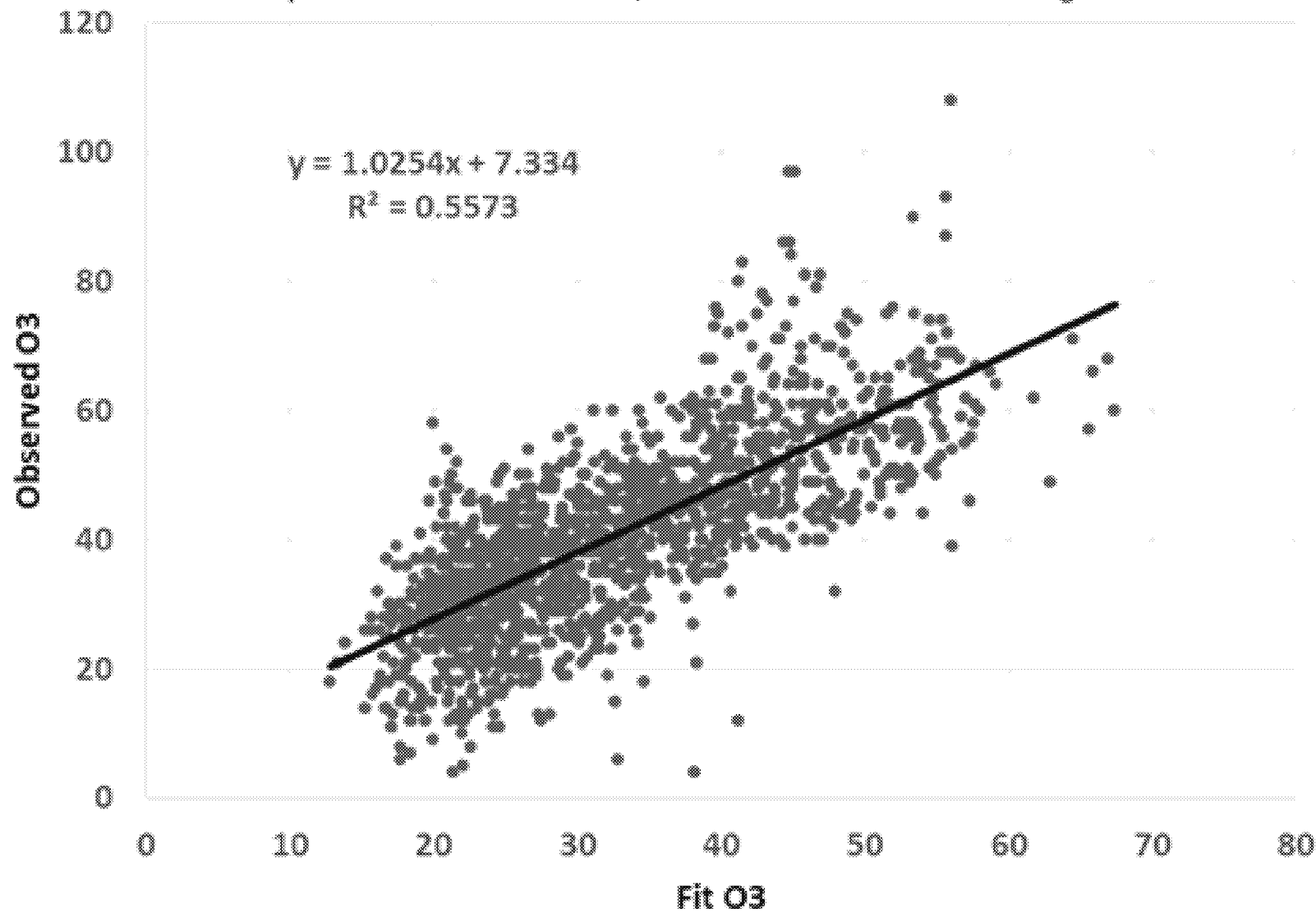
Observed vs modeled for daytime only (Hours 10am-2pm inclusive)



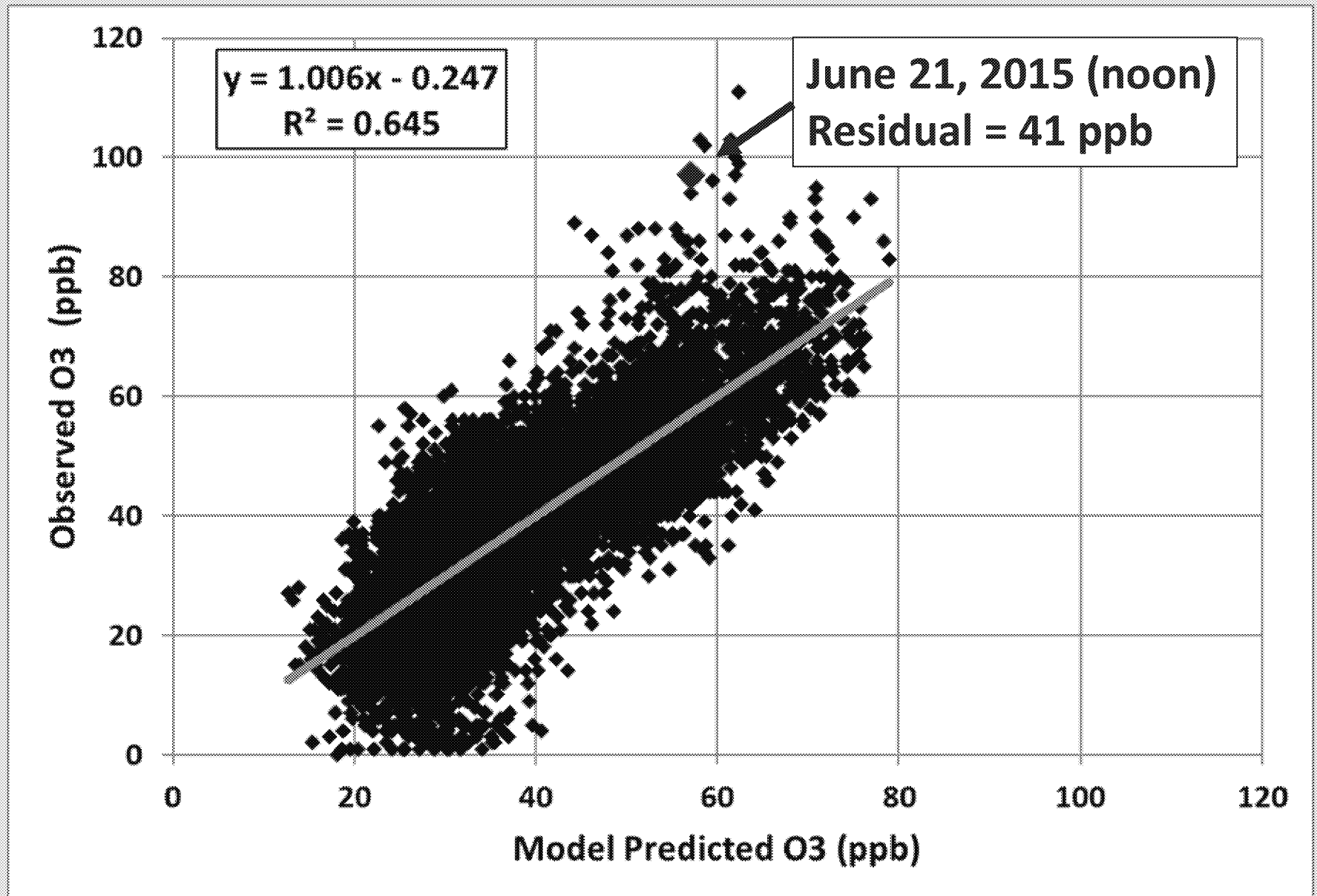
Residuals for daytime only



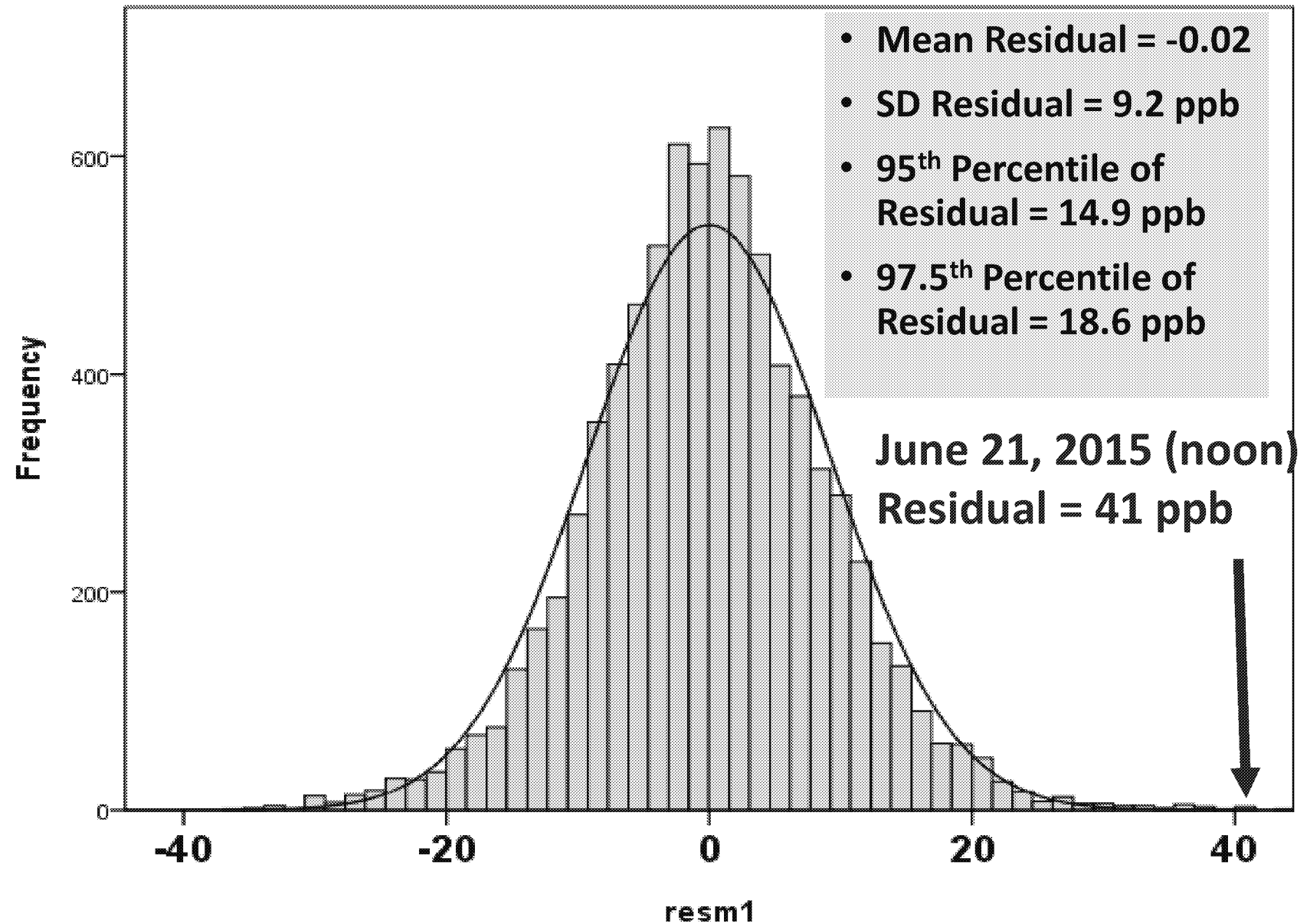
Model performance for 2015 data, when 2015 is excluded from original model



Model performance



Examine model residuals



Three ways to estimate the wildfire O₃ contribution to MDA8 from GAM predicted

1) CARB 2011 Exceptional Event package method:

$$\text{Wildfire O}_3 = \text{Obs O}_3 - \text{GAM predicted}$$

2) STI 2014 method*

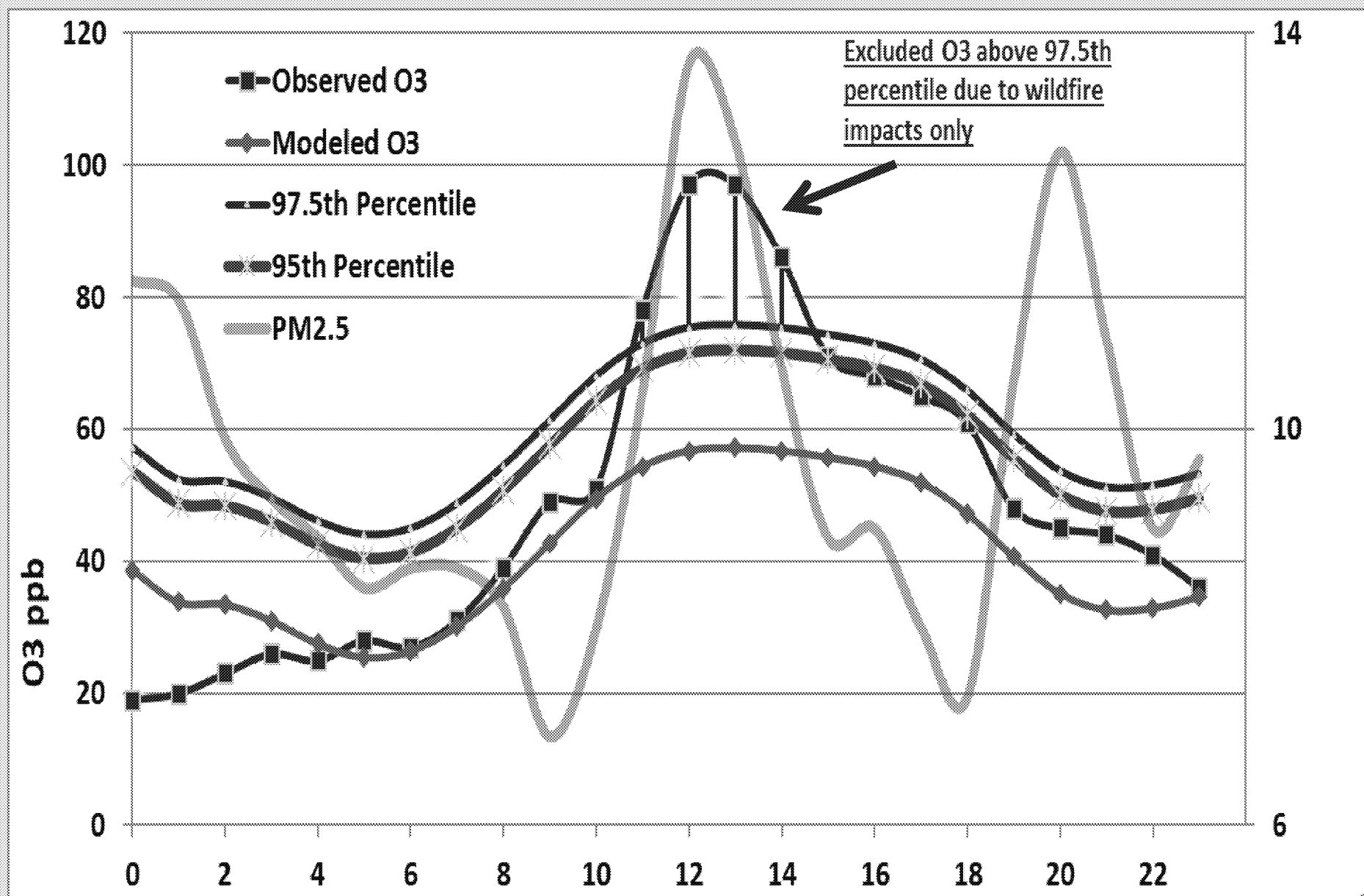
$$\text{Wildfire O}_3 = \text{Obs O}_3 - \text{GAM predicted} - \underline{95^{\text{th}} \text{ percentile value}}$$

3) EPA guidance method:

$$\text{Wildfire O}_3 = \text{Obs O}_3 - \text{GAM predicted} - \underline{97.5^{\text{th}} \text{ percentile value}}$$

*STI Technical Memorandum to EPA: Documentation of Data Portal and Case Study to Support Analysis of Fire Impacts on Ground-Level Ozone Concentrations. STI-910507-6062

**Exclude hourly O₃ above 95th (STI) or 97.5th percentile (EPA)
Adjusted MDA8 = 68 ppb (STI) or 70 ppb (EPA)**



Three ways to estimate the wildfire O₃ contribution to MDA8 from GAM predicted

CARB 2011 Exceptional Event package method:

$$\begin{aligned}\text{Wildfire O}_3 &= \text{Obs O}_3 - \text{GAM predicted} \\ &= 77 - 54 = 23 \text{ ppb}\end{aligned}$$

STI 2014 method:

$$\begin{aligned}\text{Wildfire O}_3 &= \text{Obs O}_3 - \text{GAM predicted} - 95^{\text{th}} \text{ percentile value} \\ &= 77 - 68 = 9 \text{ ppb}\end{aligned}$$

EPA guidance method:

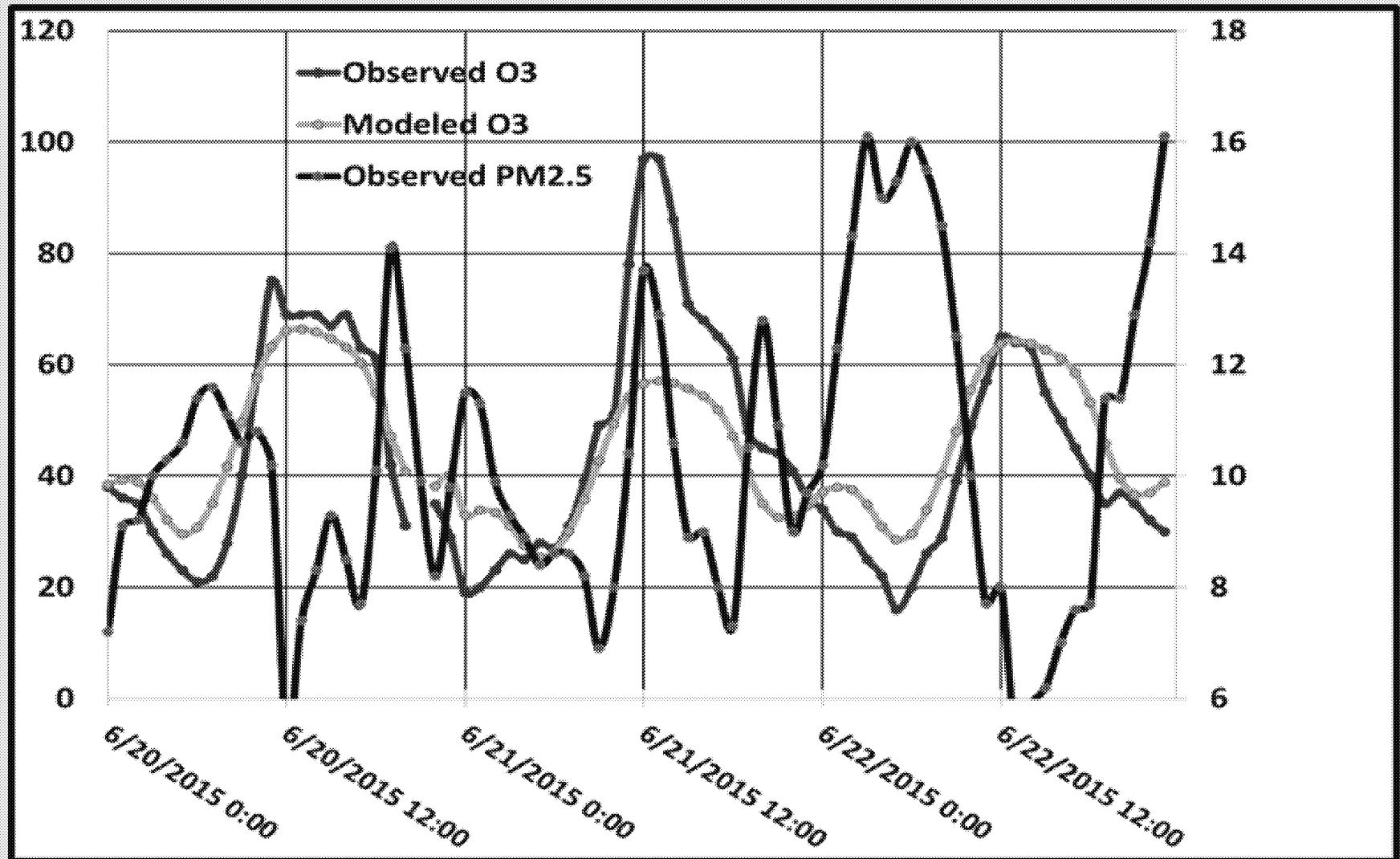
$$\begin{aligned}\text{Wildfire O}_3 &= \text{Obs O}_3 - \text{GAM predicted} - 97.5^{\text{th}} \text{ percentile value} \\ &= 77 - 70 = 7 \text{ ppb}\end{aligned}$$

Summary

1. Many factors support transport of smoke and O₃ from wildfires to El Paso UTEP site on June 21, 2015:
 - a) TCEQ demonstration (trajectories, satellite data, obs data, etc)
 - b) CAMx modeling
 - c) Pattern of enhanced PM in the daytime
 - d) Correlation of PM and O₃ (only high O₃ day in 2010-2015 with significant positive correlation)
 - e) Enhancement ratio of PM-O₃ consistent with literature values
2. Statistical modeling can be used to estimate O₃ for typical meteorological patterns. The model has an R² value of 0.64 and is tested to ensure it is unbiased.
3. Based on the statistical modeling, I estimate that the wildfires contributed 23 ppb to the MDA8 at the UTEP site on June 21, 2015. This is similar to the method used in the approved CARB 2011 Exceptional Event demonstration package.
4. Using the STI 2014 and EPA guidance methods we can estimate the minimum contributions to the MDA8 due to the wildfires of 9 ppb and 7 ppb, respectively.

Spares in case questions come up

Matching Day Analysis



Matching Day Analysis

	6/20/2015	6/21/2015	6/22/2015
Observed MDA8	67	77	56
Modeled MDA8	63	54	61
Obs - Modeled MDA8	+4	23	-5
Trajectory quadrant (after 24 hrs)	SE	SW	SE
Vector averaged wind direction for hours 10-17 (deg)	268	200	129
Trajectory distance (after 24 hours transport, km)	388	372	325
TMAX (F)	103.0	102.0	103.0
TAVG (F)	88.5	90.2	89.2
TMIN previous night (F)	77.0	77.0	75.0
DPAVG (F)	49.7	44.3	51.8
SLP AVG (mbar)	1006.4	1006.4	1007.5
Wind speed between hours 0-17 (kts)	4.0	3.6	3.2
Time of max PM	7 pm	12 pm (noon)	3 am and 11 pm



Guidance on the Preparation of Exceptional Events Demonstrations for Wildfire Events that May Influence Ozone Concentrations

Final

September 2016

EPA guidance on statistical models

Air agencies can develop the regression equation using the O₃ data for the monitor(s) under investigation and meteorology data from the closest nearby National Weather Service station. A small subset of the data should be reserved for testing the regression equation. Once a regression equation has been properly developed and tested, it can be used to predict the daily maximum O₃ values. The differences between the predicted values and the measured values are analyzed, and the 95th percentile of those positive differences (observed O₃ is greater than predicted) is recorded. This 95 percent error bound is added to the O₃ value predicted by the regression equation for the flagged days, and any difference between this sum and the observed O₃ for the flagged day may be considered an estimate of the O₃ contribution from the fire if evaluation of the top 5th percentile shows similar O₃ days in the absence of smoke are rare or not observed. !!!

See:

<https://www.epa.gov/air-quality-analysis/exceptional-events-rule-and-guidance>

EPA guidance on Q/D

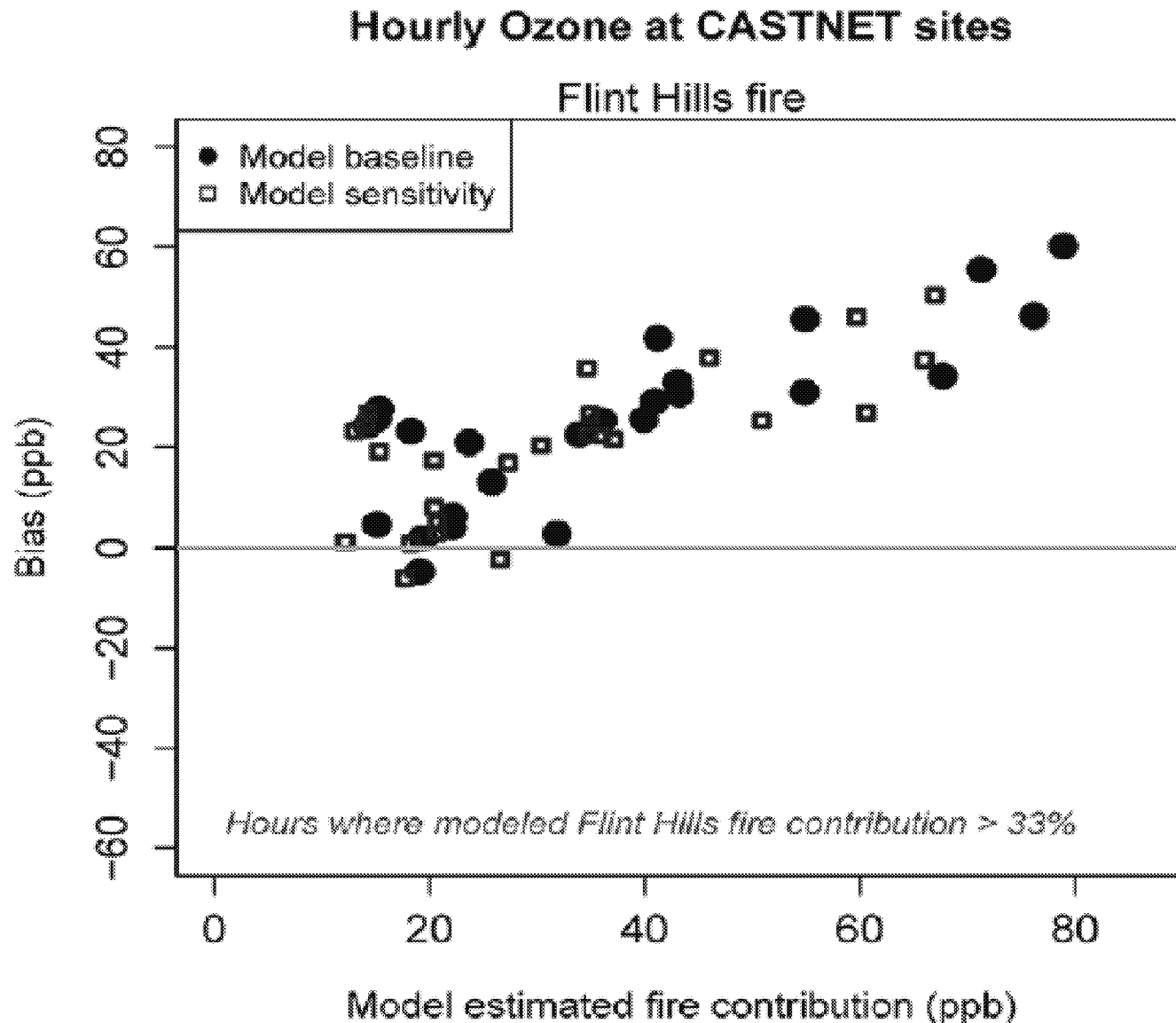
The downwind O₃ contribution from these fire events is greatest in the proximity of the fire and tends to gradually decrease as distance from the source increases. The spatial plots of downwind O₃ impacts show that the impacts occur in the direction of air mass movement from the fire event to specific places downwind. As indicated above, tiering approaches that do not explicitly account for pollutant transport (e.g., Q/D) should be accompanied with information about pollutant transport from another source such as HYSPLIT trajectories to better spatially represent the downwind impacts.

See:

<https://www.epa.gov/air-quality-analysis/exceptional-events-rule-and-guidance>

WRF model over-predictions of O₃

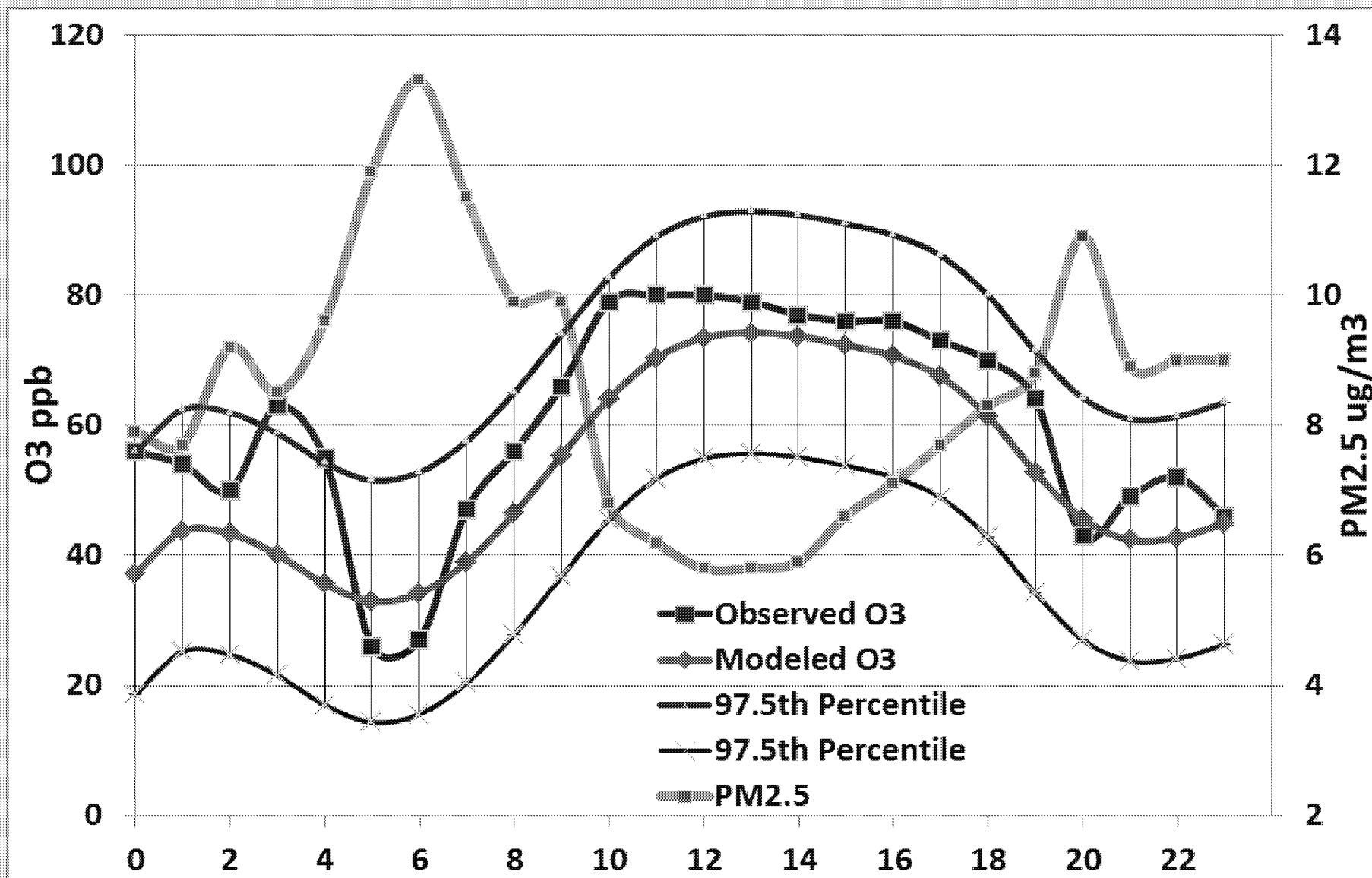
Baker et al 2016



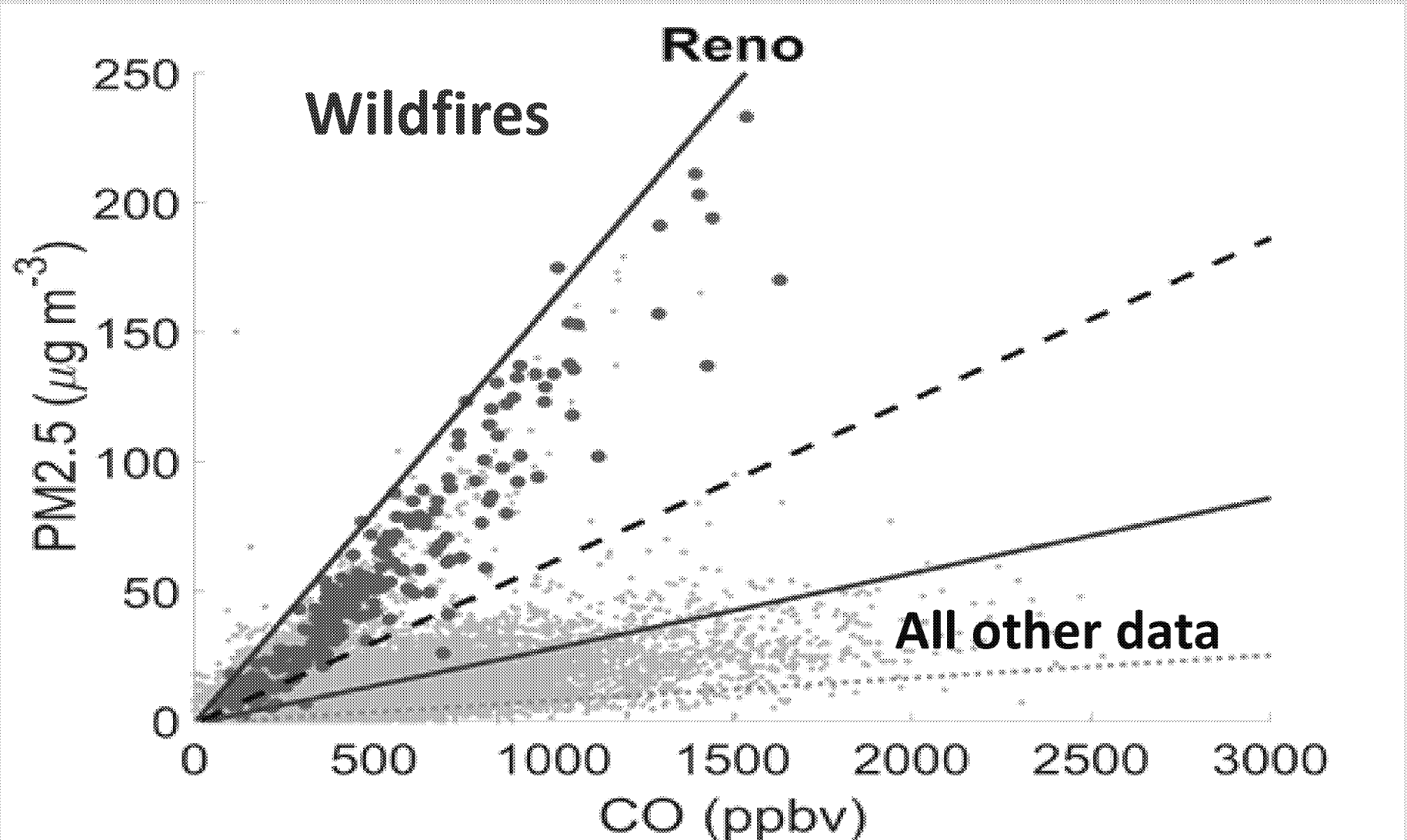
Sensitivity runs (in blue) used reduced photolysis rates, but this had little impact on over-prediction.

Baker et al.,
Contribution of regional-scale fire events to ozone and PM_{2.5} air quality estimated by photochemical modeling approaches. Atmos. Environ. 140 (2016).

July 13, 2012-corrected
Obs MDA8 = 77; Adjusted MDA8 = 77



PM_{2.5}-CO enhancement ratios for Reno



Using PM_{2.5}/CO and NO_y/CO Enhancement Ratios to Identify Wildfire Smoke Events in Western U.S. Urban Areas. (Laing and Jaffe, 2017-submitted)

Predictors for El Paso Generalized Additive Model (GAM)

Variable	Description	Source	Type C or N
TR16Q	Back-trajectory quadrant after 24 hrs	NOAA Hysplit	C
Month	Month	Month	C
WD1017	Vector averaged wind direction for Hrs 0-17	NCDC	C
Year	Year	Year	N
DOY	Day of Year	Day of Year	N
TR16D	Back-trajectory distance after 24 hrs	NOAA Hysplit	N
Hr	Hour of day	Hour of day	N
TMAX	Daily max temperature	NCDC	N
TAVG	Daily average temperature	NCDC	N
TMIN_PREV_Night	Min temperature previous night	NCDC	N
DPAVG	Daily average dew point	NCDC	N
DPMAX017	Daily maximum dew point for hours 0-17	NCDC	N
DPMIN017	Daily minimum dew point for hours 0-17	NCDC	N
SLPAVG	Daily average sea level pressure	NCDC	N
SLP017	Daily average sea level pressure for hours 0-17	NCDC	N
WS017	Vector averaged wind speed for Hrs 0-17	NCDC	N
WS617	Vector averaged wind speed for Hrs 6-17	NCDC	N
WS1017	Vector averaged wind speed for Hrs 10-17	NCDC	N